

# Polarized Fermi gases at finite temperature in the BCS-BEC crossover

Pierre-Alexandre Pantel,<sup>1</sup> Dany Davesne,<sup>1</sup> and Michael Urban<sup>2</sup>

<sup>1</sup>*Université de Lyon, Univ. Lyon 1, CNRS/IN2P3, IPN Lyon, F-69622 Villeurbanne Cedex, France*

<sup>2</sup>*Institut de Physique Nucléaire, CNRS-IN2P3 and Université Paris-Sud, 91406 Orsay Cedex, France*

We consider a polarized Fermi gas in the BCS-BEC crossover region above the critical temperature within a T matrix formalism. By treating the mean-field like shift of the quasiparticle energies in a self-consistent manner, we avoid the known pathological behavior of the standard Nozières-Schmitt-Rink approach in the polarized case, i.e., the polarization has the right sign and the spin polarizability is positive. The momentum distributions of the correlated system are computed and it is shown that, in the zero-temperature limit, they satisfy the Luttinger theorem. Results for the phase diagram, the spin susceptibility, and the compressibility are discussed.

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## I. INTRODUCTION

Initially, the crossover from the weak-coupling (BCS) superfluid phase to Bose-Einstein condensation (BEC) of molecules was mainly a theoretical idea [1–3]. Its experimental realization [4] with ultracold trapped fermionic alkali atoms, whose interaction strength (characterized by the scattering length  $a$ ) can be tuned with the help of Feshbach resonances, triggered a lot of activity from the theoretical side, not only in the context of cold atoms, but also in condensed matter and nuclear physics [5, 6]. While at zero temperature the mean-field (BCS) theory is believed to be reasonable throughout the crossover (it reproduces the correct wave function of the dimers in the BEC limit), it fails to describe the critical temperature  $T_c$ : on the BEC side,  $T_c$  is not the temperature where pairs are formed, but the temperature where the “pre-formed pairs” condense [1, 2]. By taking into account correlations above  $T_c$  in the calculation of the density, Nozières and Schmitt-Rink (NSR) obtained a theory that correctly interpolates between the BCS and BEC critical temperatures.

The situation becomes more complex if the formation of Cooper pairs is perturbed by a density or mass imbalance between the particles forming the pairs. Apart from atomic gases and superconductors in magnetic fields, such situations may be realized in nuclear matter with different densities of neutrons and protons [7, 8] or in compact stars containing light and strange quarks [9]. Such systems have been extensively studied in the recent years. For instance, one still hopes to find the Fulde-Ferrel-Larkin-Ovchinnikov (FFLO) phase with a spatially oscillating order parameter [10], which was predicted theoretically a long time ago [11, 12] but which no experiment has seen so far.

In the present work, we concentrate on the case of a uniform Fermi gas with two components (denoted by  $\sigma = \uparrow, \downarrow$  in analogy with spin-1/2 systems) having equal masses  $m$  but different densities  $\rho_\uparrow \geq \rho_\downarrow$ . Although experiments are generally done in traps, they provide information about the uniform gas under the assumption of the validity of the local-density approximation

(LDA). The experiments on the phase diagram of polarized<sup>1</sup> Fermi gases done at MIT [13–15] and Paris [16] can be well understood within the LDA. Only in an experiment at Rice University [17], clear deviations from LDA were observed, but they were later shown to correspond to a metastable non-equilibrium configuration of the atomic cloud [18, 19].

From the theoretical side, different approaches were used to describe the finite-temperature phase diagram of the polarized Fermi gas. Let us mention the quantum Monte-Carlo (QMC) calculations of Ref. [20] and the Wilsonian renormalization group approach of Ref. [21]. Also the NSR approach mentioned above was generalized to the polarized case [22]. However, it turned out that it breaks down near the unitary limit ( $a \rightarrow \infty$ ): one finds that the sign of the polarization is opposite to that of the difference between the two chemical potentials [22, 23]. Actually, there is already a problem in the unpolarized case, where the NSR approach gives a negative spin susceptibility  $\chi$  [24]. This is surprising, since a very similar approach, also based on the T matrix in ladder approximation, works very well in the extremely polarized limit at zero temperature (“polaron”) [25]. Some modified versions of the NSR scheme have been developed that avoid the unphysical behavior, such as the “extended T-matrix approximation” (ETMA) by Kashimura et al. [24] or the  $GG_0$  approach by Chen et al. [26], which was also applied to the polarized case [27, 28]. Roughly speaking, these modified versions of the NSR scheme are based on dressing a propagator line in the Feynman diagrams for the self-energy: in the ETMA, it is the upper line in Fig. 1b, while in the  $GG_0$  approach, it is one of the two lines in the ladder diagrams of Fig. 1a.

The goal of the present work is to develop a scheme similar to the NSR approach which allows us to describe the polarized Fermi gas in the normal-fluid phase from the unpolarized case above  $T_c$  up to the polaron limit. We will see that the problem of the NSR approach is

<sup>1</sup> The term “polarized” refers to a finite polarization (density imbalance) and does not imply that the gas is fully polarized.

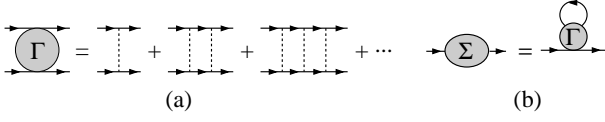


FIG. 1: Ladder diagrams for the in-medium T matrix (a) and the self-energy (b).

caused by its non-selfconsistent treatment of the quasi-particle energy shift generated by the self-energy. By simply including this shift self-consistently in *all* lines of the Feynman diagrams, the problem of the unphysical sign of the polarization is avoided. Within this framework, we will compute the phase transition line towards the paired (superfluid or FFLO) phase, the equation of state in the normal phase, and the correlated occupation numbers.

The article is organized as follows. We present the formalism in Sec. II. Then we discuss the correlated density and occupation numbers (Sec. III), the phase diagram (Sec. IV) and the compressibility and spin susceptibility (Sec. V). Finally, Sec. VI contains the summary and further discussions. Throughout the article, we use units with  $\hbar = k_B = 1$ , where  $\hbar$  and  $k_B$  denote, respectively, the reduced Planck constant and the Boltzmann constant.

## II. FORMALISM

The starting point of the NSR approach and most of its variants is the T matrix, i.e., the interaction in the medium is calculated in ladder approximation (see Fig. 1a)

$$\Gamma(\Omega, \mathbf{q}) = \left( \frac{m}{4\pi a} - J(\Omega, \mathbf{q}) \right)^{-1} \quad (1)$$

where  $\Omega$  and  $\mathbf{q}$  are energy (measured relatively to the sum of the two chemical potentials,  $\mu_\uparrow + \mu_\downarrow$ ) and momentum of the pair,

$$J(\Omega, \mathbf{q}) = \int \frac{d^3k}{(2\pi)^3} \left( \frac{1 - f(\xi_{\mathbf{k}+\mathbf{q},\uparrow}^*) - f(\xi_{\mathbf{k},\downarrow}^*)}{\Omega - \xi_{\mathbf{k}+\mathbf{q},\uparrow}^* - \xi_{\mathbf{k},\downarrow}^*} + \frac{m}{k^2} \right) \quad (2)$$

is the retarded in-medium two-particle propagator (regularized in the usual way [29]),  $\xi_{\mathbf{k}\sigma}^*$  are the quasiparticle energies (measured with respect to  $\mu_\sigma$ ), and  $f(\xi) = 1/(e^{\xi/T} + 1)$  is the Fermi function for temperature  $T$ . In the standard NSR theory [3, 29], one takes instead of  $\xi_{\mathbf{k}\sigma}^*$  the free-particle dispersion relation,  $\xi_{\mathbf{k}\sigma}^0 = k^2/(2m) - \mu_\sigma$ . In the present work, we will make a step towards a more self-consistent treatment by using a modified dispersion relation that includes interaction effects. In principle, it would be desirable to calculate  $\xi_{\mathbf{k}\sigma}^*$  by looking for the pole of the dressed Green's function, i.e., from

$$\xi_{\mathbf{k}\sigma}^* = \xi_{\mathbf{k}\sigma}^0 + \text{Re } \Sigma_\sigma(\xi_{\mathbf{k}\sigma}^*, \mathbf{k}). \quad (3)$$

In ladder approximation, the self-energy  $\Sigma_\sigma$  of a particle with spin  $\sigma$  is calculated from  $\Gamma$  by closing the line corresponding to the particle with the opposite spin,  $\bar{\sigma}$ , as shown in Fig. 1b. Calculating this diagram within the imaginary-time (Matsubara) formalism and performing the analytic continuation to real energies [30] one obtains for the imaginary part of the retarded self-energy

$$\text{Im } \Sigma_\sigma(\omega, \mathbf{k}) = - \int \frac{d^3k'}{(2\pi)^3} \text{Im } \Gamma(\omega + \xi_{\mathbf{k}'\sigma}^*, \mathbf{k} + \mathbf{k}') \times [f(\xi_{\mathbf{k}'\bar{\sigma}}^*) + g(\omega + \xi_{\mathbf{k}'\sigma}^*)], \quad (4)$$

where  $g(\omega) = 1/(e^{\omega/T} - 1)$  denotes the Bose function. The real part can be obtained from the imaginary part with the help of a dispersion relation,

$$\text{Re } \Sigma_\sigma(\omega, \mathbf{k}) = -\mathcal{P} \int \frac{d\omega'}{\pi} \frac{\text{Im } \Sigma_\sigma(\omega', \mathbf{k})}{\omega - \omega'}. \quad (5)$$

Within the original NSR theory [3, 29], the density is obtained from the thermodynamic potential in ladder approximation. This is equivalent to calculating the density from the Green's function obtained by truncating the Dyson equation at first order, i.e.,  $G_\sigma = G_\sigma^0 + G_\sigma^{02} \Sigma_\sigma$  [26], where  $G_\sigma^0 = 1/(\omega - \xi_{\mathbf{k}\sigma}^0)$  denotes the non-interacting Green's function. As a consequence, the density for each spin state has two contributions,  $\rho_\sigma = \rho_\sigma^{(0)} + \rho_\sigma^{(1)}$ , where  $\rho_\sigma^{(0)}$  is the density of an ideal Fermi gas with chemical potential  $\mu_\sigma$ , and the correction  $\rho_\sigma^{(1)}$  is given by

$$\rho_\sigma^{(1)} = \frac{\partial}{\partial \mu_\sigma} \int \frac{d^3q}{(2\pi)^3} \int \frac{d\Omega}{\pi} g(\Omega) \delta(\Omega, \mathbf{q}), \quad (6)$$

where

$$\delta(\Omega, \mathbf{q}) = -\text{Im } \ln \left( J(\Omega, \mathbf{q}) - \frac{m}{4\pi a} \right) \quad (7)$$

is the in-medium scattering phase shift. In the presence of a bound state ( $a > 0$ ), one has  $\delta = \pi$  in the energy range between the bound-state energy and the continuum threshold.

In other variants of the NSR theory, the Dyson series has been resummed to all orders, i.e.,  $G_\sigma = 1/(\omega - \xi_{\mathbf{k}\sigma}^0 - \Sigma_\sigma)$  [31]. In either way,  $\Sigma_\sigma$  describes at the same time correlation effects and a mean-field like shift of the single-particle energies.

In the present work, the situation is slightly different. The bare lines correspond already to quasiparticle Green's functions  $G_\sigma^* = 1/(\omega - \xi_{\mathbf{k}\sigma}^*)$  that contain the modified dispersion relation  $\xi_{\mathbf{k}\sigma}^*$ . The mean-field like shift is thus included self-consistently (also in the calculation of  $\Gamma$ ). The additional correlation effects are responsible for the  $\omega$ -dependence of  $\Sigma_\sigma$ . To first order in the correlations, we therefore get

$$G_\sigma(\omega, \mathbf{k}) = G_\sigma^*(\omega, \mathbf{k}) + G_\sigma^{*2}(\omega, \mathbf{k}) [\Sigma_\sigma(\omega, \mathbf{k}) - \text{Re } \Sigma_\sigma(\xi_{\mathbf{k}\sigma}^*, \mathbf{k})]. \quad (8)$$

Using this approximation, one can express the occupation numbers  $n_{\mathbf{k}\sigma}$  in the form  $n_{\mathbf{k}\sigma} = n_{\mathbf{k}\sigma}^{(0)} + n_{\mathbf{k}\sigma}^{(1)}$  as a sum of the uncorrelated occupation numbers  $n_{\mathbf{k}\sigma}^{(0)} = f(\xi_{\mathbf{k}\sigma}^*)$  and a correction due to correlations

$$n_{\mathbf{k}\sigma}^{(1)} = \int \frac{d\omega}{\pi} \text{Im} \Sigma_{\sigma}(\omega, \mathbf{k}) \frac{f(\xi_{\mathbf{k}\sigma}^*) - f(\omega)}{(\omega - \xi_{\mathbf{k}\sigma}^*)^2}. \quad (9)$$

Accordingly, the densities are again a sum of uncorrelated and correlated densities,  $\rho_{\sigma} = \rho_{\sigma}^{(0)} + \rho_{\sigma}^{(1)}$ , but now  $\rho_{\sigma}^{(0)}$  is the density of an uncorrelated gas of quasiparticles with dispersion relation  $\xi_{\mathbf{k}\sigma}^*$ . After some algebra, the expression for the correction  $\rho^{(1)}$  can be reduced to

$$\rho^{(1)} = - \int \frac{d^3q}{(2\pi)^3} \int \frac{d\Omega}{\pi} g'(\Omega) \left( \delta - \frac{1}{2} \sin(2\delta) \right). \quad (10)$$

Note that, in contrast to Eq. (6), in the present approach the correlated density  $\rho^{(1)}$  is independent of the spin  $\sigma$ . This is plausible since a correlated pair consists of one atom of each spin. The expression (10) for the correlated density was originally derived for the unpolarized case by Zimmermann and Stolz (ZS) in Ref. [32] in a condensed-matter context and subsequently used in Refs. [5, 33, 34] to describe the BEC-BCS crossover in nuclear matter.

For practical reasons, in order to simplify the numerical calculations, we make an additional approximation: we replace the momentum dependent shift  $\text{Re} \Sigma_{\sigma}(\xi_{\mathbf{k}\sigma}^*, \mathbf{k})$  in the quasiparticle energies  $\xi_{\mathbf{k}\sigma}^*$  by a constant shift  $U_{\sigma}$ , calculated at the respective Fermi surface,  $k_{F\sigma} = (6\pi^2 \rho_{\sigma})^{1/3}$ , i.e., we use

$$\xi_{\mathbf{k}\sigma}^* \approx \xi_{\mathbf{k}\sigma}^0 + U_{\sigma}, \quad \text{with} \quad U_{\sigma} = \text{Re} \Sigma_{\sigma}(\xi_{k_{F\sigma}}^*, k_{F\sigma}). \quad (11)$$

With this approximation, the T matrix  $\Gamma$  and the self-energies  $\Sigma_{\sigma}$  are identical to those of the standard T-matrix approximation if one replaces the chemical potentials  $\mu_{\sigma}$  by “effective” ones

$$\mu_{\sigma}^* = \mu_{\sigma} - U_{\sigma}. \quad (12)$$

Actually, as long as one is not interested in the “real” chemical potentials  $\mu_{\sigma}$ , it is not necessary to compute the shift  $U_{\sigma}$  and all calculations can be done as functions of  $\mu_{\sigma}^*$ . However, the shift  $U_{\sigma}$  is needed if one is interested in the relation between the densities  $\rho_{\sigma}$  and the real chemical potentials  $\mu_{\sigma}$ .

### III. CORRELATED DENSITIES AND OCCUPATION NUMBERS

As we discussed before, the main difference between the mean-field approach on the one hand and the NSR and ZS approaches on the other hand is the inclusion of pair correlations above  $T_c$  in the calculation of the density. If we consider a sufficiently strong asymmetry of the densities or chemical potentials, we can calculate the correlation correction to the density as a function of

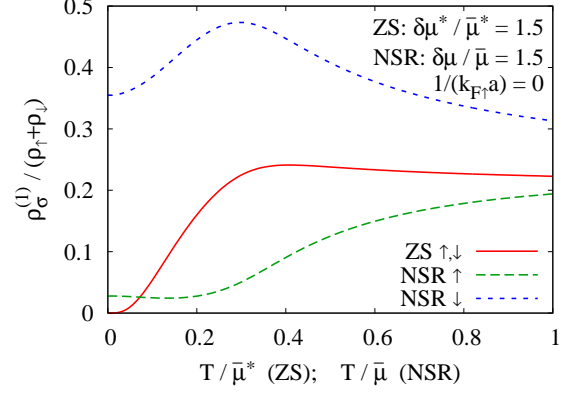


FIG. 2: Temperature dependence of the correlation correction to the densities within the present (ZS) approach (solid line) compared with the corrections to the majority (long dashes) and minority (short dashes) densities within the original NSR approach.

temperature down to  $T = 0$  without ever reaching the superfluid phase. As an example, we show in Fig. 2 the temperature dependence of the correction to the density,  $\rho^{(1)}$ , obtained within the present approach (ZS) and the temperature dependence of the corrections  $\rho_{\sigma}^{(1)}$  obtained within the original NSR approach, normalized to the total density  $\rho_{\uparrow} + \rho_{\downarrow}$ , in the unitary limit. In the NSR case, we kept the chemical potentials  $\mu_{\uparrow, \downarrow} = \bar{\mu} \pm \delta\mu/2$  constant, with  $\delta\mu = 1.5\bar{\mu}$ , whereas in the ZS case, we fixed for simplicity the effective chemical potentials  $\mu_{\uparrow, \downarrow}^*$ .

One sees that the behaviors of the spin-independent correction  $\rho^{(1)}$  in the ZS case and of the spin-dependent ones,  $\rho_{\sigma}^{(1)}$ , in the NSR case are qualitatively different: in the ZS case, the correction vanishes in the limit of zero temperature. In contrast, in the NSR scheme, the correction  $\rho_{\sigma}^{(1)}$  does not only account for correlations, but also for the mean-field like shift of quasiparticle energies (which within the ZS scheme is included in the effective chemical potentials  $\mu_{\sigma}^*$ ). Since the minority atoms ( $\downarrow$ ) feel a much stronger attractive “mean field” than the majority atoms ( $\uparrow$ ), the NSR correction  $\rho_{\downarrow}^{(1)}$  is much larger than  $\rho_{\uparrow}^{(1)}$ , and both corrections remain finite at  $T = 0$ .

The fact that within the ZS approach  $\rho^{(1)} \rightarrow 0$  for  $T \rightarrow 0$  is directly related to the Luttinger theorem [35]. This theorem states that, at  $T = 0$ , the relationship between the density  $\rho_{\sigma}$  and the Fermi momentum (i.e., the momentum where the occupation numbers are discontinuous),  $\rho_{\sigma} = k_{F\sigma}^3 / (6\pi^2)$ , remains unchanged even though correlations modify the occupation numbers. Since this relation is already fulfilled with the uncorrelated occupation numbers  $n_{\mathbf{k}\sigma}^{(0)} = \theta(k_{F\sigma} - k)$ , this implies that the integral of the correction  $n_{\mathbf{k}\sigma}^{(1)}$ , i.e.,  $\rho^{(1)}$ , must vanish at  $T = 0$ . Our numerical results show that this is indeed the case. It is interesting to notice that by including the shift  $U_{\sigma}$  self-consistently, one apparently recovers in the  $T \rightarrow 0$  limit the results of the  $T = 0$  formulation of the so-called

“particle-particle random-phase-approximation”, where one starts from the beginning with Green’s function that depend on  $k_{F\sigma}$  and not on  $\mu_\sigma$  [36].

Let us now have a look at the occupation numbers themselves. In Fig. 3 we show the occupation numbers for  $\uparrow$  and  $\downarrow$  atoms in the unitary limit for a given polarization  $P = (\rho_\uparrow - \rho_\downarrow)/(\rho_\uparrow + \rho_\downarrow) = 0.85$  for three different temperatures. Let us first discuss the case of  $T = 0.5T_F$  (right panel). At first glance, the change between uncorrelated ( $n_{\mathbf{k}\sigma}^{(0)}$ ) and correlated ( $n_{\mathbf{k}\sigma}$ ) occupation numbers seems to be very small in this case. One sees that  $n_{\mathbf{k}\sigma}$  is slightly reduced at small  $k$  and slightly enhanced at large  $k$  as compared with  $n_{\mathbf{k}\sigma}^{(0)}$ . However, the main effect becomes visible if we look at the asymptotic high-momentum tail shown in the inset. The correlated occupation numbers ( $n_{\mathbf{k}\sigma}$ ) fall off like  $1/k^4$ , the coefficient being the same for both spins, while the uncorrelated ones ( $n_{\mathbf{k}\sigma}^{(0)}$ ) decrease of course exponentially.

At a lower temperature,  $T = 0.3T_F$  (central panel), we see in addition to the increase of the correlated occupation numbers at high momenta a sizeable reduction at low momenta, especially for the minority component. This fits into the common picture of how correlations modify the occupation numbers at  $T = 0$ : particles are scattered out of the Fermi sea, which reduces the occupation numbers below  $k_{F\sigma}$  and leads to a finite occupancy of states above  $k_{F\sigma}$ . In the present case, the Fermi surfaces are of course washed out by the finite temperature.

As it was already pointed out in Ref. [36], the fact that the pairs are always formed of one  $\uparrow$  and one  $\downarrow$  atom implies that, at  $T = 0$ , the depletion of the particle number inside the Fermi sphere is the same for both spins, i.e., the occupation numbers of the minority ( $\downarrow$ ) species are necessarily more strongly reduced than those of the majority species ( $\uparrow$ ). As we see, this effect persists at finite temperature.

At even lower temperature,  $T = 0.1T_F$  (left panel), we observe that the correlation correction to the minority occupation numbers becomes so strong that the occupation numbers  $n_{\mathbf{k}\downarrow}$  become negative. This is of course unphysical and shows the limits of the perturbative treatment of the correlations, i.e., of the truncation of the Dyson series at first order in the self-energy in Eq. (8). The same problem was found in Ref. [36]. However, as soon as one goes more towards the BCS side of the crossover, this problem appears only at very low temperatures and very close to the critical polarization.

#### IV. PHASE DIAGRAM

Before we consider the phase diagram of the polarized gas, let us briefly discuss the unpolarized case and compare our results with those of the original NSR theory. As in the NSR approach [29], the critical temperature is determined from the Thouless criterion  $\Gamma^{-1}(0, 0) = 0$ ,

i.e.,

$$J(0, 0) = \frac{m}{4\pi a}, \quad (13)$$

but now,  $J$  is calculated with the chemical potential  $\mu^* = \mu_\uparrow^* = \mu_\downarrow^*$  (in the unpolarized case we can drop the spin indices) and the corresponding density is obtained from the ZS formula (10). In Fig. 4, we display the critical temperature  $T_c$  in units of the Fermi energy  $E_F = k_F^2/(2m)$  as function of the dimensionless parameter  $1/(k_F a)$  characterizing the interaction strength. For the solid line,  $k_F$  was calculated with the density corrected by the ZS formula (10), while the dashed line was obtained with the standard NSR correlated density [29].

Both theories interpolate between the mean-field (BCS) result (corresponding to  $\rho = \rho^{(0)}$  without correction; dotted line) in the limit  $1/(k_F a) \rightarrow -\infty$  and the condensation temperature for an ideal gas of bosonic molecules in the limit  $1/(k_F a) \rightarrow \infty$  (BEC, dash-dotted line). However, we see that on the side  $1/(k_F a) < 0$ , the ZS formula reaches the BCS limit much faster than the NSR one, which gives  $T_c^{\text{NSR}} < T_c^{\text{BCS}}$  even for relatively weak interactions. This reduction of  $T_c^{\text{NSR}}$  in the weak-coupling regime looks similar to the Gor’kov-Melik-Barkhudarov (GMB) correction [37] to  $T_c^{\text{BCS}}$ , however its origin is completely different: while the GMB correction is due to screening of the interaction in the medium, the reduction of  $T_c^{\text{NSR}}$  comes from the non self-consistent treatment of the mean-field like shift in the original NSR theory.

Coincidentally, the critical temperatures obtained with the ZS and NSR formulas in the unitary limit ( $1/(k_F a) = 0$ ) are very close to each other ( $T_c/E_F \approx 0.23$ ). Although they are much lower than the BCS result ( $T_c^{\text{BCS}}/E_F \approx 0.5$ ), they are still too high because of missing screening effects: recent experimental values range from  $T_c/E_F = 0.157(15)$  [16] to  $0.167(13)$  [38].

On the BEC side ( $a > 0$ ), the ZS critical temperature goes through a minimum before it rises again and approaches the BEC limit, whereas the NSR critical temperature goes through a maximum. Qualitatively, the NSR behavior is in better agreement with QMC results [20] than the ZS one. The presence of a minimum in the ZS critical temperature seems to be a general property of this approach, cf. the results in the literature for nuclear matter [5, 33, 34].

Let us now turn to the polarized case. Again, the critical temperature (or polarization) is determined by the appearance of a pole in the T matrix at  $\omega = 0$ , but in the polarized case it may happen that the pole appears first (for decreasing temperature or polarization) at a finite value of  $\mathbf{q}$ , corresponding to the transition to a FFLO-like phase [22]. Therefore the condition to be in the normal phase reads:

$$J(0, \mathbf{q}) > \frac{m}{4\pi a} \quad \text{for all } \mathbf{q}. \quad (14)$$

As mentioned in the introduction, the standard NSR theory presents in the polarized case a pathology near

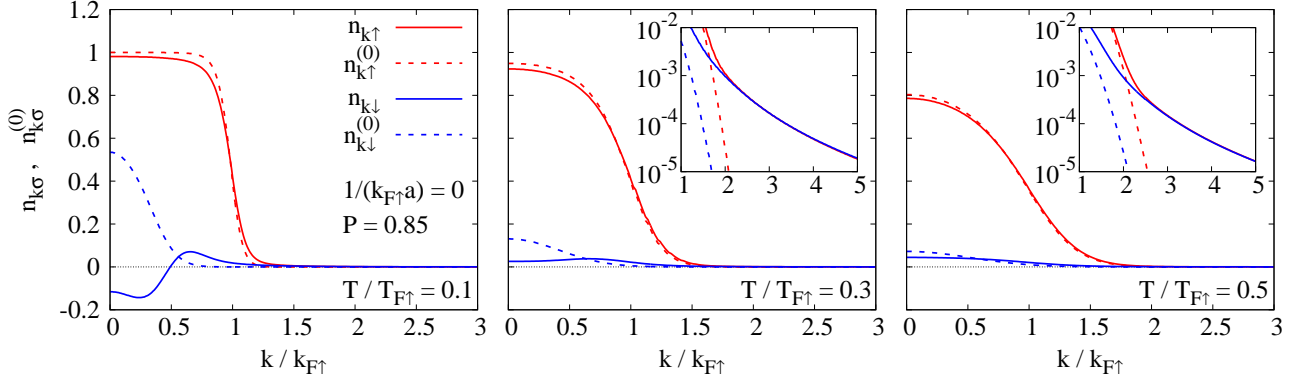


FIG. 3: Momentum dependence of the occupation numbers in the unitary limit for polarization  $P = 0.85$  and three different temperatures  $T/T_F = 0.1, 0.3$ , and  $0.5$  (from left to right). The insets show the asymptotic high-momentum tail of the occupation numbers on a logarithmic scale. The upper (red) curves represent the occupation numbers of the majority ( $\uparrow$ ) atoms, while the lower (blue) lines represent those of the minority ( $\downarrow$ ) atoms. The solid lines are the correlated occupation numbers  $n_{k\sigma}$  while the dashed lines represent the uncorrelated ones  $n_{k\sigma}^{(0)}$ .

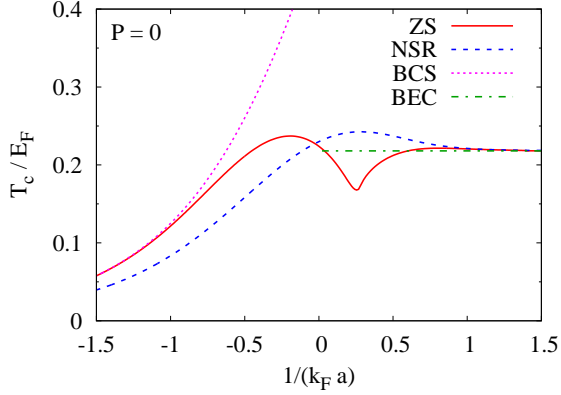


FIG. 4: Critical temperature  $T_c$  in units of  $E_F$  vs. the dimensionless parameter  $1/(k_F a)$  characterizing the interaction strength for the unpolarized gas. Solid line: present approach (ZS), dashes: NSR result, dots: BCS result, dash-dots: BEC limit.

the unitary limit: for  $\mu_\uparrow > \mu_\downarrow$ , one finds  $\rho_\uparrow < \rho_\downarrow$  in large regions of the phase diagram [22, 23]. To illustrate this problem we show in Fig. 5 the phase diagram obtained within the NSR scheme for  $1/(k_F a) = 0$ . The pathology is present in the gray shaded region delimited by the dotted line. Since the pathology extends down to  $\delta\mu = 0$ , it implies that the spin susceptibility of the unpolarized gas is negative in some temperature range above  $T_c$  [24]. As we will see, the self-consistent treatment of the shift  $U_\sigma$  in our approach cures these problems.

Let us discuss the phase diagram within our approach as function of temperature  $T$  and polarization  $P = (\rho_\uparrow - \rho_\downarrow)/(\rho_\uparrow + \rho_\downarrow)$ . The phase diagrams for two different values of the interaction strength,  $1/(k_F a) = 0$  and  $-0.5$ , are shown in Figs. 6 and 7, respectively. The solid and dashed lines indicate the results obtained for the critical temperature  $T_c$  within the generalized ZS scheme, while the dotted lines are mean-field results, i.e., what

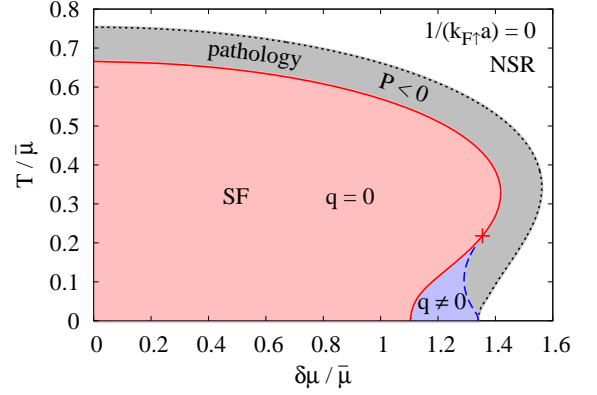


FIG. 5: Phase diagram of the unitary Fermi gas obtained within the standard NSR scheme as function of temperature  $T$  and difference of the chemical potentials  $\delta\mu$ , both normalized by the average chemical potential  $\bar{\mu}$ . The solid line indicating the transition towards a BCS- (or Sarma-) like superfluid (SF) phase is obtained with the usual Thouless criterion (13), whereas the dashed line accounts for the possibility of a FFLO-like phase with a finite momentum  $\mathbf{q} \neq 0$  of the Cooper pairs, cf. Eq. (14). In the region delimited by the dotted line, the NSR approach presents a pathology in the sense that the polarization has the wrong sign.

one obtains if one neglects the correlation contribution  $\rho^{(1)}$  to the density. The cross marks the tricritical point where the phase transition is not longer towards the ordinary BCS-like superfluid or Sarma phase ( $\mathbf{q} = 0$ ) but towards a FFLO-like phase ( $\mathbf{q} \neq 0$ ). Since our formalism does not allow us to calculate the densities inside the superfluid phase, we cannot draw the line separating these phases.

In both cases,  $1/(k_F a) = 0$  and  $-0.5$ , we checked that the difference between the real chemical potentials,  $\delta\mu$ , is always positive for  $P > 0$ , i.e., the pathology of the NSR scheme is not present here.

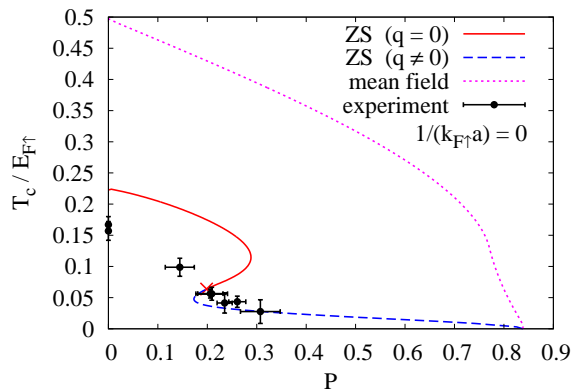


FIG. 6: Critical temperature  $T_c$  in units of  $E_{F\uparrow} = k_{F\uparrow}^2/(2m)$  vs. polarization  $P$  for a unitary Fermi gas ( $1/(k_{F\uparrow}a) = 0$ ). The transition towards a BCS- (or Sarma-) like superfluid is shown as the solid line, while the dashed line indicates a transition towards a FFLO-like phase. The cross marks the tricritical point separating BCS, FFLO, and normal phase. For comparison, the  $T_c$  vs.  $P$  curve obtained without the correction  $\rho^{(1)}$  (BCS mean-field result) is shown as the dotted line. The experimental data are from Shin et al. [15] except the points at  $P = 0$  which are from Nascimbène et al. [16] ( $T_c/T_F = 0.157(15)$ ) and Ku et al. [38] ( $T_c/T_F = 0.167(13)$ ).

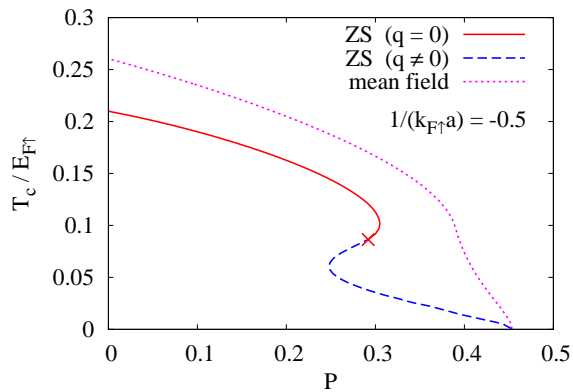


FIG. 7: Same as Fig. 6 but for  $1/(k_{F\uparrow}a) = -0.5$ .

One sees that in the case  $1/(k_Fa) = -0.5$  (Fig. 7), the BCS mean-field result clearly differs from that of the full calculation, but the difference is not dramatic. If one goes further to the BCS regime [ $1/(k_Fa) < -1$ ], the BCS mean-field and full calculations give practically identical results. However, as mentioned before, one should be aware of the fact that BCS mean-field theory as well as our calculation miss corrections due to screening of the in-medium interaction. Therefore it seems likely that not only our critical temperatures, but also the critical polarizations are too high.

In the unitary limit (Fig. 6), the inclusion of the correlated density  $\rho^{(1)}$  changes the phase diagram completely, as expected from our results discussed above for the unpolarized case. Again, compared with the results of the

MIT and ENS experiments [15, 16, 38], the critical temperature  $T_c$  we obtain at small polarization  $P$  is still too high because of missing screening effects.

In the region of lower temperature and higher polarization ( $P \gtrsim 0.2$ ), the experiment found a first-order phase transition (phase separation), while we get a second-order phase transition towards the FFLO phase in this region. We cannot check whether there is a first-order phase transition since this requires to compare the energies of the paired and the unpaired phases, the former being inaccessible within our formalism. But it is clear that, if there was a first-order phase transition, the critical polarization would have to be higher than the one where we find the second-order phase transition.

At very low temperature, the critical polarization increases a lot and exceeds by far the experimental one. Actually, in our formalism, the critical polarization beyond which the system stays in the normal phase even at  $T = 0$  (Chandrasekhar-Clogston limit) is the same as the one obtained in mean-field theory. The reason for this is that, as discussed in the preceding section, the correlated density  $\rho^{(1)}$  vanishes in the  $T \rightarrow 0$  limit, as required by the Luttinger theorem. This high value of the critical polarization is probably due to the uncorrelated occupation numbers  $n_{\mathbf{k}\sigma}^{(0)}$  in Eq. (2), which are almost step functions at low temperature. Maybe a more self-consistent treatment of correlations, i.e., the inclusion of correlated occupation numbers  $n_{\mathbf{k}\sigma}$  in Eq. (2), could improve the results. In nuclear physics, such an approach is known as “renormalized random-phase approximation” [39, 40], but it is beyond the scope of this work.

## V. SPIN SUSCEPTIBILITY AND COMPRESSIBILITY

By considering a very small polarization, we can determine the spin susceptibility of the unpolarized gas. To be precise, the spin susceptibility is defined as [24]

$$\chi = \lim_{\delta\mu \rightarrow 0} \frac{\rho_{\uparrow} - \rho_{\downarrow}}{\delta\mu}. \quad (15)$$

Note that for the computation of  $\delta\mu$  (not  $\delta\mu^*$ ) one needs the self-energy, cf. Eq. (11). In Fig. 8, we show the temperature dependence of the spin susceptibility for  $1/(k_{F\uparrow}a) = 0$  (solid line), in units of the spin susceptibility of an ideal Fermi gas at zero temperature,  $\chi_0(T = 0) = mk_F/(2\pi^2)$ . First of all, we see that  $\chi$  is positive, which is already a good point. For comparison, the temperature dependence of the susceptibility of an ideal Fermi-gas,  $\chi_0$ , is shown, too (dotted line). It seems plausible that the susceptibility  $\chi$  of the correlated system is lower than that of the ideal gas,  $\chi_0$ , because the pairs made of  $\uparrow$  and  $\downarrow$  atoms resist against polarization. Similar results were obtained by Kashimura et al. [24] within the ETMA (dashes). Very surprisingly, the experimental results for  $\chi$  [41] are close to  $\chi_0$  or even higher. However, one should notice that these



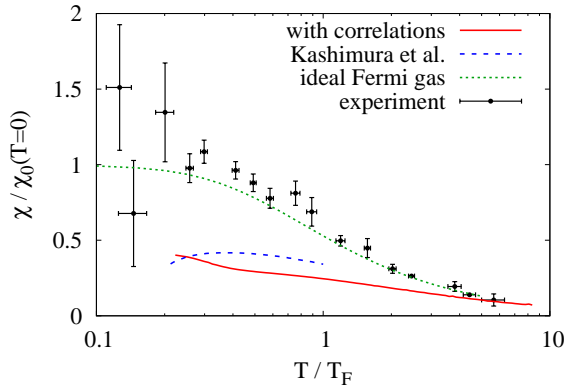


FIG. 8: Spin susceptibility (normalized to the susceptibility of an ideal Fermi gas at  $T = 0$ ) of the unpolarized unitary Fermi gas as a function of temperature. The experimental data are taken from Sommer et al. [41].

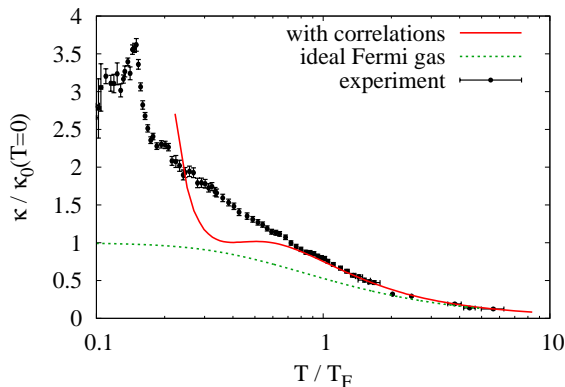


FIG. 9: Compressibility (normalized to the compressibility of an ideal Fermi gas at  $T = 0$ ) of the unpolarized unitary Fermi gas as a function of temperature. The experimental data are taken from Ku et al. [38] (for  $T/T_F < 2$ ) and from Sommer et al. [41] (for  $T/T_F > 2$ ).

data were determined very indirectly from a complicated non-equilibrium situation.

Although not related to the polarized Fermi gas, we can also study the compressibility of the unpolarized gas above  $T_c$ . Following Ref. [41], the compressibility is defined as  $\kappa = (\partial\rho/\partial\mu)/\rho^2$ , where  $\rho = \rho_\uparrow = \rho_\downarrow$  is the density per spin state. Again, the computation of  $\kappa$  requires both the correlated density and the self-energy. Our results for  $\kappa$ , normalized by the susceptibility of an ideal Fermi gas at zero temperature,  $\kappa_0(T=0) = 3/(2E_F\rho)$ , are shown in Fig. 9 together with the ideal Fermi-gas result  $\kappa_0$  and the experimental data from Refs. [38, 41]. We observe that the compressibility is higher than that of the ideal Fermi gas, which is plausible for a system with attractive interaction. For  $T \gtrsim 0.8T_F$ , our results agree very well with the experimental ones. At lower temperatures, the nice agreement is lost. When  $T$  approaches  $T_c$  from above, a strong increase of the compressibility is found in both theory and experiment. However, since

our  $T_c$  is too high, we find this increase at a higher temperature than observed in experiment.

## VI. SUMMARY AND DISCUSSION

Although very successful in the description of the BCS-BEC cross-over of an unpolarized two-component Fermi gas, the Nozières-Schmitt-Rink (NSR) approach fails in the case of finite polarization  $P$ . As it was already pointed out in previous work [22–24], the NSR scheme gives in some regions of the phase diagram  $\rho_\uparrow < \rho_\downarrow$  in spite of  $\mu_\uparrow > \mu_\downarrow$ , and even in the unpolarized case the spin susceptibility has the wrong (negative) sign.

In this work we have suggested a way how to overcome the problems of the original NSR approach in the polarized case. As in the NSR scheme, we start from the ladder approximation for the  $T$  matrix and the single-particle self-energy  $\Sigma_\sigma$ . We split  $\Sigma_\sigma$  into a constant mean-field like shift  $U_\sigma$  and an energy-dependent part describing the correlations. While the correlations are treated perturbatively, the shift  $U_\sigma$  is included self-consistently. This is different from the original NSR approach, where the self-energy  $\Sigma_\sigma$  as a whole is included only to first order in the truncated Dyson series. We retrieve a well-known formula for the correlation correction to the density, originally derived by Zimmermann and Stolz (ZS) [32] for the unpolarized case.

Within the ZS scheme, the correlation correction to the density,  $\rho^{(1)}$ , does not depend on the spin, which is plausible since the correlated pairs are made of one atom of each spin. Another interesting property of this approach is that  $\rho^{(1)}$  vanishes in the limit  $T \rightarrow 0$ , as required by the Luttinger theorem. Apparently, by including the energy shift  $U_\sigma$  one recovers in the  $T \rightarrow 0$  limit the results of the particle-particle random-phase approximation formulated within the  $T = 0$  formalism [36].

When calculating occupation numbers, one finds that near unitarity and at low temperature, the correlations become too strong to be treated perturbatively. Apparently in these cases one cannot avoid to sum the Dyson series to all orders, as it was done, e.g., in Refs. [24, 31]. This is beyond the scope of this work and it is also not clear whether such a resummation would respect, e.g., the equality of the correlation densities of both spins and the Luttinger theorem in the  $T \rightarrow 0$  limit.

In the unpolarized case, the ZS approach interpolates, as the NSR approach, between the BCS and BEC limits, however it reaches the BCS limit much faster than the NSR approach. Near the unitary limit, the critical temperatures for a given density are much lower than the BCS one but still too high because screening effects of the Gor'kov-Melik-Barkhudarov type [37] are not included.

In contrast to the NSR scheme, the ZS scheme allows us to calculate the phase diagram also as a function of polarization, since the polarization has the same sign as the difference between the chemical potentials, as it should. At not too strong polarizations, the generalized ZS ap-

proach predicts a second-order phase transition towards a BCS- or Sarma-like superfluid phase. At higher polarization and lower temperature, one finds instead a transition towards a FFLO-like phase where the Cooper pairs have a finite momentum. This is in contrast to the experimental results obtained in the unitary limit [15] which show a first-order phase transition with phase-separation between normal and superfluid phases at high polarization and low temperature. In order to study a possible first-order transition theoretically, one would need a theory that describes both the normal and the superfluid phase. Another problem is the critical polarization for the transition towards the FFLO phase at  $T = 0$ , which is much too high in our approach.

The spin susceptibility of the unpolarized gas within our approach is positive, as it should be. It is smaller than that of an ideal Fermi gas, which is also plausible. It agrees more or less with the theoretical prediction of the extended T matrix approximation (ETMA) [24] and of the Luttinger-Ward theory [42], but not with the ex-

perimental results of Ref. [41].

It should be noted that, even though the self-consistent energy shift is a first step into that direction, one is still very far from a fully self-consistent scheme such as that of Ref. [42, 43] where all lines in Fig. 1 would correspond to dressed Green's functions. A less ambitious improvement would be the so-called renormalized RPA [39, 40] which amounts to replacing in Eq. (2) the Fermi functions  $f(\xi_{\mathbf{k}\sigma}^*)$  by the self-consistent occupation numbers  $n_{\mathbf{k}\sigma}$ . This would probably reduce the strong correlations, especially at low temperature, and therefore help to reduce the critical polarization of the FFLO phase.

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